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(FILE 'HOME' ENTERED AT 17:39:52 ON 22 SEP 2005)

FILE 'CA' ENTERED AT 17:40:00 ON 22 SEP 2005

E ADAMY S/AU

L1 3 S E4-7 AND 1994/PY

L2 6988 S (CONTOUR OR (3 OR THREE) (2W) DIMENSION?) (7A) (PLOT? OR DIAGRAM OR REPRESENT? OR DISPLAY OR GRAPH?)

L3 1179 S L2 AND (PHASE OR W O OR O W OR EMULSI? OR MICROEMULS? OR (WATER OR H2O) (1A) OIL OR SUSPENSION)

L4 117 S L3 AND (AUTOMAT? OR COMPUTER OR MICROPROCESSOR)

L5 111 S L4 NOT (COMPRESS? OR MICROPORE OR ORIFICE OR ION CHROMATOG? OR CHEMICAL FORMULA OR TOMOGRAPHY OR WAVE FORM OR COMBINATORI?)

L6 81 S L5 NOT (VIRUS OR REFRACT? OR DIGEST? OR MINING OR COLONY OR HOLOGR? OR ARTS OR PREDICT? OR DIMER)

L7 72 S L6 NOT (VOID OR POLYANIL? OR YEAST OR PROTEIN OR SOIL OR CYTOPLASM OR ENZYM? OR LIGAND OR POCKET OR INTERATOM? OR CEMENT)

L8 56 S L7 NOT (DIFFRACT? OR BIOINF? OR ANNULAR OR POSTING OR CHANNEL OR FLAME OR ESTROGE? OR ANNEAL? OR PLANT OR AMYLOID)

L9 61 S L4 NOT L8

L10 1 S L9 AND STYRENE

L11 57 S L8, L10

=> d bib, ab 1-3 11

L1 ANSWER 2 OF 3 CA COPYRIGHT 2005 ACS on STN

AN 121:303582 CA

TI Effects of cosurfactant and oil chain length on phase behavior and solubilization in alcohol and glycol ether microemulsions

AU Adamy, S. T.

CS Technology Center, Colgate-Palmolive Company, Piscataway, NJ, 08855, USA

SO Journal of Dispersion Science and Technology (1994), 15(6), 727-48

AB The phase behavior and oil solubilization capacities of a series of model microemulsion systems have been studied. Phase behavior was studied in systems composed of NaCl brine, sodium dodecyl sulfate, and either 1-butanol, 1-pentanol, ethylene glycol monobutyl ether, diethylene glycol monobutyl ether, ethylene glycol monohexyl ether, or diethylene glycol monohexyl ether. Longer-chained cosurfactant systems exhibit isotropic behavior over smaller compositional ranges. Whereas the ethylene glycol monohexyl ether system possessed two sep. isotropic microemulsion-type regions, all other systems possessed connected isotropic regions. The one-phase regions in the 1-pentanol system, however, are connected by a narrow channel. Increasing the degree of amphiphilicity in the cosurfactant tends to increase the occurrence of liq. crystal phases. The effects of changing the cosurfactant structure and the oil chain length in oil solubilization were also analyzed. We introduce the method of presenting solubilization data in the form of contour plots, and demonstrate the utility of these plots for understanding solubilization. It was generally found in both alc. and glycol ether systems that lengthening the cosurfactant chain or shortening the oil chain tended to increase solubilization and drive the systems to be more dependent on the amt. of cosurfactant and less on the amt. of surfactant. In the ethylene glycol monohexyl ether system, liq. crystals could be formed when octane or dodecane was solubilized and

high concns. of amphiphiles were present, but not when hexadecane was solubilized. The trends in solubilization were able to be qual. described by Winsor's R ratio anal., which may provide a means of performing direct calcns. to predict behavior in these systems.

=> d bib,ab 1-57 115

L11 ANSWER 32 OF 57 CA COPYRIGHT 2005 ACS on STN
AN 112:166184 CA
TI Phase equilibrium calculations and **three-dimensional computer graphics representation**
AU Nitta, Tomoshige; Ikeda, Kazufumi; Katayama, Takashi
CS Fac. Eng. Sci., Osaka Univ., Osaka, 560, Japan
SO Fluid Phase Equilibria (1989); 53, 105-12
AB An important role of global stability anal. is emphasized for **phase** equil. calcns. to det. the thermodynamically most stable soln. An algorithm used in this work is to find first an outside soln. in the Gibbs energy surface and then to search any inside solns. by means of the bisection search principle. The global stability anal. should also be applied to mixt. crit. points calcd. from the conventional crit. condition. Typical **phase** diagrams are calcd. for binary mixts. including three **phases** (gas, liq. and solid) by using the Soave-Redlich-Kwong equation of state. **Three-dimensional** pressure-temp.-comprn. (pTx) **phase diagrams** were displayed on a personal **computer** with functions of rotation, zoom, enlargement and projections on the pT, px and Tx axes.

L11 ANSWER 47 OF 57 CA COPYRIGHT 2005 ACS on STN
AN 98:34972 CA
TI Mathematical treatment of the **emulsification** of benzene and **styrene** in aqueous hexadecyltrimethylammonium bromide-cetyl alcohol mixtures
AU Chou, Y. J.; El-Aasser, M. S.; Vanderhoff, J. W.
CS Emulsion Polymers Inst., Lehigh Univ., Bethlehem, PA, 18015, USA
SO ACS Symposium Series (1982), 197(Comput. Appl. Appl. Polym. Sci.), 399-425
AB **styrene** [100-42-5] Or benzene [71-43-2] mini-**emulsions** of 0.1-0.3 μ diam. were prep'd. at 63° using a mixt. of aq. hexadecyltrimethylammonium bromide (I) [57-09-0] and cetyl alc. [36653-82-4]. The most stable **emulsions**, formed at 1:3-1:1 molar ratios, contained cryst., rodlike particles of I and II, 1-2 μ in length and 0.1-0.2 μ in diam. Conductometric titrn. of these optimum systems with **styrene** or benzene gave a near-linear leg descending to an inflection point followed by another near-linear leg ascending to a second inflection point and a near-const. or slowly-decreasing leg thereafter. The descending leg was interpreted as solubilization of the oil in micelles or cryst. complex, the ascending leg as **emulsification** to form tiny droplets which grew by coalescence and diffusion, and the near-const. or slowly decreasing leg to droplet growth by diffusion. The conductometric titrn. curves were expressed by an exponential step function in terms of the initial conductance, the conductances at both inflection points, a solubilization const., an **emulsification** const., and a droplet growth const. Iterative **computer** soln. of this math. model gave a reasonable fit of the different exptl. titrn. curves, and the calcd. parameters were correlated with the I and II concns. to give the distributions of

the **emulsifier** as solute **emulsifier**, micellar **emulsifier**, and **emulsifier** in the cryst. complex. The correlation of **emulsion** stability with the presence of the cryst., rodlike particles allowed a prediction of **emulsion** stability. Finally, a **three-dimensional plot** of conductance as a function of added benzene and II concn. at a given I concn. was calcd. by **computer** curve-fitting and used to visualize the conductance surface at any desired angle.

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(FILE 'HOME' ENTERED AT 16:22:09 ON 22 SEP 2005)

FILE 'CA' ENTERED AT 16:22:33 ON 22 SEP 2005

L1 4895 S (3 OR THREE) (2W) DIMENSION? (7A) (PLOT? OR DIAGRAM OR CONTOUR OR
REPRESENT? OR DISPLAY OR GRAPH?)
L2 359 S L1(10A) (AUTOMAT? OR COMPUTER)
L3 33 S L2 AND (PHASE OR W O OR O W OR EMULSI? OR MICROEMULS? OR (WATER OR
H2O) (1A) OIL)
L4 228 S L2 AND GRAPHIC?
L5 74 S L4 AND (EXPERIMENT OR DATA)
L6 104 S L3, L5
L7 94 S L6 NOT (COMPRESS? OR MICROPORE OR ORIFICE OR ION CHROMATOG? OR
CHEMICAL FORMULA OR TOMOGRAPHY OR WAVE FORM OR COMBINATORI?)
L8 71 S L7 NOT (VIRUS OR REFRACT? OR DIGEST? OR MINING OR COLONY OR HOLOGR?
OR ARTS OR PREDICT? OR DIMER)
L9 43 S L8 NOT (VOID OR POLYANIL? OR YEAST OR PROTEIN OR SOIL OR CYTOPLASM
OR ENZYM? OR LIGAND OR POCKET OR INTERATOM? OR CEMENT)
L10 32 S L9 NOT (DIFFRACT? OR BIOINF? OR ANNULAR OR POSTING OR CHANNEL OR
FLAME OR ESTROGE? OR ANNEAL? OR PLANT OR AMYLOID)

=> d 110 bib,ab 1-32

L10 ANSWER 13 OF 32 CA COPYRIGHT 2005 ACS on STN

AN 115:44115 CA

TI Investigation of emulgation and **emulsion** stability of thiocarbamate
herbicides

AU Dombay, Zs.; Mogyorodi, F.

CS North Hung. Chem. Works, Sajabolony, H-3792, Hung.

SO Proc. Conf. Colloid Chem. Mem. Ervin Wolfram, 5th (1990), Meeting Date
1988, 106-9. Editor(s): Kiss, E.; Pinter, J. Publisher: Lorand Eotvos
Univ., Budapest, Hung.

AB **Emulsification** and **emulsion** stability (persistence in time) of
thiocarbamate herbicides (ethiolate, EPTC, cycloate and butylate) were
investigated through photometric measurement of turbidity. Influence of
various parameters was evaluated. Investigations included combined
herbicidal formulations. Results were analyzed and **represented** by
computer in **three-dimensional diagrams**.

L10 ANSWER 15 OF 32 CA COPYRIGHT 2005 ACS on STN

AN 114:120915 CA

TI PlotIT - **graphics** and statistics in 3 dimensions

AU Schweim, Harald; Nagel, Klaus
CS Inst. Pharm. Chem., Univ. Hamburg, Hamburg, D-2000/13, Germany
SO Pharmazie in Unserer Zeit (1991), 20(1), 37-41
LA German
AB The personal computer version (1.5) of the **data** processing, statistical evaluation, and **data graphical** display program PlotIT, was critically tested for its applicability for chem.-related **data** processing and representation on an IBM-compatible with a 80386 processor. The program, which is either command- or menu-driven and which enables the 3-dimensional representation of histogram or X/Y/Z plots ("fish net" plots) in addn. to conventional X/Y plots, histograms, or pie charts, performed well; 1 or 2 minor errors were apparent (e.g. default parameters which could lead to a system crash). These are described, together with the various functions of the program. The program requires hardware corresponding to its high std.; this, coupled with its complexity which requires a certain amt. of familiarization probably makes it more suitable for large, rather than small, labs.

L10 ANSWER 20 OF 32 CA COPYRIGHT 2005 ACS on STN
AN 106:127893 CA
TI Modular software-controlled electrochemical system
AU Hagan, D.; Spivey, J.; Niculescu, V. A.
CS Virginia Commonw. Univ., Richmond, VA, 23284-0001, USA
SO Review of Scientific Instruments (1987), 58(3), 468-74
AB A modular microcomputer-controlled 3-electrode potentiostat configured with **graphics** is presented. The system was designed for metallic surface characterization and is capable of performing in different modes of operation including single sweep voltammetry, cyclic voltammetry, and chronoamperometry. An integrated and flexible software system for control, **data** taking, **data** storage, and transfer is described. **Data** anal. software for the IBM-PC **computer** including 2- and 3-dimensional **plotting** as well as menu-driven theor. modeling, simulation, and curve fitting was developed.

L10 ANSWER 24 OF 32 CA COPYRIGHT 2005 ACS on STN
AN 103:148098 CA
TI Three-dimensional PTx **phase diagrams** through interactive **computer graphics**
AU Charos, Georgios N.; Clancy, Paulette; Gubbins, Keith E.; Naik, Chandrashekhar D.
CS Sch. Chem. Eng., Cornell Univ., Ithaca, NY, 14853, USA
SO Fluid Phase Equilibria (1985), 23(1), 59-78
AB Interactive computer graphic techniques were developed for the display of binary mixt. **phase diagrams**. The diagrams are defined in temp.-pressure-comprn. space, and are pictured as wireframe objects with depth perception in order to provide a three-dimensional effect. The displays used were vector refresh workstations whose transformation hardware allows real-time rotation, rescaling, and translation of the diagrams, while software allows the extn. of const. property Px, Tx, PT, and x-y plots. The equil. surfaces and the crit. lines were calcd. by using the Redlich-Kwong equation of state and its Soave modification.

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